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Development of a Nonperiodic Homogenization Method for One-Dimensional Continua

by Michael J. Leamy, Peter W. Chung, and Raju Namburu

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Michael J. Leamy
U.S. Military Academy

Peter W. Chung and Raju Namburu
Computational and Information Sciences Directorate, ARL

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*Assistant Professor, U.S. Military Academy, Department of Mechanical Engineering, West Point, NY 10996.
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14. ABSTRACT

This work describes a one-dimensional homogenization method that relaxes the usual assumption of periodicity of microscale displacements. As such, this method is appropriate for studying materials with periodic as well as nonperiodic microstructures. Expected applications for the new method include composite rods with manufacturing variability (where material periodicity is destroyed) and rods composed of functionally graded materials. The method is validated through direct comparison with a known exact solution, that being a rod with linearly varying axial rigidity. The method for this case is shown to be exact. Further application of the developed method to two different periodic materials is used to validate the usual periodic assumption employed in traditional homogenization methods.

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1. Introduction

The traditional asymptotic homogenization method has found wide acceptance in the composites modeling community (Bendsoe and Kikuchi, 1988; Fish et al., 1999; Francfort and Murat, 1986; Ghosh et al., 1996; Hollister et al., 1994; Lene, 1986; Moulinec and Suquet, 1998; Sanchez-Palencia, 1980; Shkoller and Hegemier, 1995), for its ability to incorporate and estimate effective material properties from a subscale representative unit cell (Babuska, 1976). Central to the method is the principal of convergence, which has been studied in the mathematical literature for H-, G-, Γ-, and two-scale convergence. In simple terms, H-convergence, for example, states that over an open bounded domain Ω in R^N, a sequence of bounded and finite matrices A^{ε} is said to H-converge to a sequence of bounded and finite matrices A if, for all $f \in H^{-1}(\Omega)$, the solution u^{ε} of $-div(A^{\varepsilon}\nabla u^{\varepsilon}) = f$, $u^{\varepsilon} \in H_0^1(\Omega)$ converges, as the scaling parameter ε goes to zero, in weak-$H_0^1(\Omega)$ to the solution u of $-div(A\nabla u) = f$, $u \in H_0^1(\Omega)$ and if the sequence $A^{\varepsilon}\nabla u^{\varepsilon}$ converges in weak-$L^2(\Omega)^N$ to $A\nabla u$. In general, the H-limit of A^{ε}, which is A, is not explicit except under certain assumptions. The works of Bensoussan et al. (1978) and Sanchez-Palencia (1980) are commonly cited to show that the explicit H-limit is known for periodic systems. Loosely speaking, for the convergence of A^{ε} in the appropriate space of linear operators, or the convergence of the Green's operator, the literature refers to G-convergence (Spagnolo, 1976). The convergence of $\left(A^{\varepsilon}\nabla u^{\varepsilon}, \nabla u^{\varepsilon}, u^{\varepsilon}\right)$ is referred to as Γ-convergence (Tartar, 1978), and a more specific case of H-convergence, which takes into account the periodicity of the solution, is referred to as two-scale convergence (Allaire, 1992).

The engineering and computational mechanics literature have made such extensive use of these fundamental mathematical developments that it is difficult to provide a truly exhaustive bibliography. We note among many, however, the work on structural optimization (Bendsoe and Kikuchi, 1988), biomechanics (Hollister et al., 1994), and multiphysics solid mechanics (Fish et al., 1999; Fish and Yu, 2001; Ghosh et al., 1996, 2001; Lene, 1986; Moulinec and Suquet, 1998; Shkoller and Hegemier, 1995; Terada et al., 2000; Terada and Kikuchi, 2001). Until now, however, the engineering developments in homogenization have mainly considered specialized cases of two-scale convergence where the periodicity is built into the computational procedure. The application of the so-called y-periodicity generally precludes the ability to consider nonperiodic systems. In this regard, developments in the engineering and mathematical literature have been on divergent paths.

We have found that nonperiodicity can occur under two scenarios. The first is when the finite boundary has a direct influence on the solution, or the reduction-of-dimension situation, which can occur typically in laminated plates or stratified rods. The second is when the material exhibits finite microstructure but in a nonperiodic sense. This can commonly be encountered in the form of localized behavior, such as that found in damage mechanics or fracture, or in smoothly varying microscopic material dependence on macroscopic coordinates, such as that found in functionally graded composites.

Limited works by the engineering community have attempted to modify the homogenization method for systems involving finitely thick plates (Rostam-Abadi et al., 2000). Still others have considered the presence of strong anharmonic local fields that disrupt the periodicity and require increased resolution solutions (Oden and Vemaganti, 1999; Ghosh et al., 2001; Oden et al., 2001). In these works, the traditional periodic homogenization method has been modified at a schematic level using the laminated plate theory (Rostam-Abadi et al., 2000) or *h* and *p* finite element adaptivity techniques (Ghosh et al., 2001; Oden et al., 2001) so that directions in Cartesian space or regions within a nonperiodically deforming body are specifically accounted for by small changes in the periodic homogenization procedure. On the other hand, developments in the mathematical literature have been tied to special cases where material dependence on spatial coordinates is strictly demonstrable (Briane, 1994; Shkoller, 1997; Fabre and Mossino, 1998). Namely, they consider material types where key heterogeneous features are within a diffeomorphic mapping and linear mapping away from a periodic arrangement.

Briane (1994) developed a nonperiodic homogenization method in which a highly oscillatory but nonperiodic matrix A^{ε} is compared to a periodic matrix B^{ε} as the microscale feature size goes (slower) to zero as ε goes to zero. The limit of B^{ε} is a function of every point in the material. Recognizing the computationally infeasible nature of this approach, Shkoller (1997) showed that the problem could be simplified to a unit cell approach, where the microscale feature size is kept finite and the error in the approximation is of the order of the unit cell size. In this sense, the asymptotic nature of homogenization is not being fully assumed. Fabre and Mossino (1998) completed a similar study, looking at H-convergent multiplicable matrices that may be used to perform a linear mapping that takes a periodic material into a nonperiodic one thereby allowing periodic homogenization of a mapped nonperiodic material. Gustafsson and Mossino (2003) developed a nonperiodic homogenization method for diffusion equations based on the H-convergent multiplicable matrices of Fabre and Mossino (1998) to write explicit expressions of homogenization for a plate and less explicit expressions for a thin cylinder.

Developments in nonperiodic homogenization stem from the general H-convergence properties of the homogenization theory combined with mapping principles and dimension reduction. In its most general and primitive form, homogenization makes no presumption of periodicity, which indicates that its application to nonperiodic systems can be made forthwith. Bensoussan et al. (1978) have shown a one-dimensional result for homogenization that is implicit in its absence of periodicity constraints on the microstructure.

In this report, we develop a one-dimensional nonperiodic computational homogenization method with explicit equations and show that it recovers the periodic case. This is done by relaxing the periodicity assumption of the microscale displacement field, integrating analytically, and applying a boundedness argument to the result. The procedure is entirely different from that of

Bensoussan et al. (1978) yet is shown to yield the same result. This enables the development of the new computational homogenization procedure for the one-dimensional continua (i.e., for the elastic rod). Generalization to the three-dimensional continua is expected to follow in a later paper. When compared to the engineering literature, the procedure described differs in two ways: (1) the approximation space is introduced early in the procedure, and (2) no periodicity condition is imposed on the microscale displacement field. This second difference is expected to make the new procedure relevant to a wider class of problems than the preceding homogenization procedures. Using the example of an end-displaced rod with linearly varying axial rigidity *EA*, a comparison is made between the displacement field predicted by the new homogenization procedure and the displacement field of the exact solution. A second example of a rod with periodically varying axial rigidity is used to discuss the appropriateness of the microscale periodicity condition imposed by preceding homogenization procedures.

2. On a New Homogenization Procedure

2.1 Formulation

Consider a straight rod characterized by an axial rigidity *EA*, whose deformation is described by a displacement field $u^{\varepsilon}(x^{\varepsilon})$ governed by the equilibrium equation

$$\frac{\partial}{\partial x^{\varepsilon}}\left(EA\frac{\partial u^{\varepsilon}}{\partial x^{\varepsilon}}\right)=-f\,, \tag{1}$$

where for the simplicity of discussion, the external forcing f will be considered to be absent. Consider further the rod to be fixed rigidly at its initiating end with a prescribed displacement at its terminating end:

$$u^{\varepsilon}(x^{\varepsilon}=0)=0, \tag{2}$$

and

$$u^{\varepsilon}(x^{\varepsilon}=l)=u_{l}\,. \tag{3}$$

This choice of end conditions is motivated by an eventual finite element implementation of the described procedure, in which the end conditions take the form of equations 2 and 3, and a rigid body translation. The axial rigidity *EA* of the described rod is considered to be nonuniform. It can be decomposed into a constant macroscale axial rigidity and a nonconstant microscale axial rigidity

$$EA=EA^{0}+EA^{1}(y)\,, \tag{4}$$

where dependence on the macroscale implies $x = x^{\varepsilon}$ dependence and dependence on the microscale implies $y = x^{\varepsilon}/\varepsilon$ dependence, ε being a small parameter. The equilibrium equation can be updated to reflect dependence on the two scales by using the derivative expression

$$\frac{\partial}{\partial x^{\varepsilon}} = \frac{\partial}{\partial x} + \frac{1}{\varepsilon}\frac{\partial}{\partial y}. \tag{5}$$

As in previous homogenization procedures, the displacement field is expanded using ε:

$$u^{\varepsilon}(x^{\varepsilon}) = u^{0}(x,y) + \varepsilon u^{1}(x,y) + \cdots, \tag{6}$$

where $u^{0}(x,y)$ and $u^{1}(x,y)$ denote macro- and microscale displacement fields, respectively. Interchangeably, $u^{0}(x,y)$ will be termed the $O(\varepsilon^{0})$ displacement, where $O(\,)$ denotes the order operator, and $u^{1}(x,y)$ will be termed the $O(\varepsilon^{1})$ displacement. Introducing equations 5 and 6 into equation 1 while neglecting quantities of $O(\varepsilon^{2})$ in equation 6, followed by a separation of orders of ε, yields the following governing equations:

for ε^{-2},

$$\frac{\partial}{\partial y}\left(EA\frac{\partial u^{0}}{\partial y}\right) = 0; \tag{7}$$

for ε^{-1},

$$\frac{\partial EA}{\partial y}\left(\frac{\partial u^{0}}{\partial x} + \frac{\partial u^{1}}{\partial y}\right) + 2EA\frac{\partial^{2} u^{0}}{\partial x \partial y} + EA\frac{\partial^{2} u^{1}}{\partial y^{2}} = 0; \tag{8}$$

for ε^{0},

$$\frac{\partial EA}{\partial y}\frac{\partial u^{1}}{\partial x} + EA\frac{\partial^{2} u^{0}}{\partial x^{2}} + 2EA\frac{\partial^{2} u^{1}}{\partial x \partial y} = 0; \tag{9}$$

and for ε^{1},

$$EA\frac{\partial^{2} u^{1}}{\partial x^{2}} = 0. \tag{10}$$

Without loss of generality, the boundary inhomogeneity u_{l} is *not* expanded and the boundary conditions can be restated as

$$u^{0}(0,0) = 0, \tag{11}$$

$$u^{1}(0,0) = 0, \tag{12}$$

$$u^{0}(l, l/\varepsilon) = u_{l}^{0}, \tag{13}$$

and

$$u^1(l, l/\varepsilon) = 0\,. \tag{14}$$

Integrating equation 7 twice with respect to *y* yields

$$u^0(x,y) = C_1(x)\alpha(y) + C_2(x)\,, \tag{15}$$

where $\alpha(y) = \int \frac{1}{EA}dy$. Assuming $C_1(x)$ is not proportional to ε, so as to preserve the relative ordering of all terms in (equation 6) for all *y*, the presence of $\alpha(y)$ in equation 15 results in $u^0(x,y)$ being unbounded as $y \to \infty$, or equivalently then, as $\varepsilon \to 0$. For example, retaining only the macroscale term in the axial rigidity for ease of explanation, at the terminal end $\alpha(y = l/\varepsilon)$ evaluates to $\frac{1}{\varepsilon}\frac{l}{EA^0}$, which is unbounded as $\varepsilon \to 0$. We require that the solution procedure be bounded, or appealing to a physical argument, be applicable to the case of a homogenous rod where ε is arbitrarily small, in which case, the need for a bounded $u^0(x,y)$ requires that $C_1(x)$ be zero.

To further facilitate a solution, an approximating space is introduced for $C_2(x)$. Specifically, we search for an approximation to $u^0(x,y)$ such that $C_2(x) \in H^1(x)$ (i.e., the Sobolev space of degree 1) (Hughes, 1987). For simplicity herein, a single element that spans the rod's length *l* will be considered, but, more generally, the use of the H^1 Sobolev approximation space admits usage of multiple elements while insuring displacement continuity across the element boundaries. In accordance with this discussion, a linear polynomial approximation for $C_2(x)$ is introduced:

$$C_2(x) = a_2 x + b_2\,, \tag{16}$$

where a_2 and b_2 are unknown constants. Applying the boundary conditions (equations 11 and 13) yields

$$u^0(x,y) = u^0(x) = \frac{u_l^0}{l}x\,. \tag{17}$$

With the determination of the $O(\varepsilon^0)$ displacement completed, the analysis of the $O(\varepsilon^1)$ displacement follows. Substituting equation 17 into equations 8, 9, and 10 yields

$$\frac{\partial EA}{\partial y}\left(\frac{u_l^0}{l} + \frac{\partial u^1}{\partial y}\right) + EA\frac{\partial^2 u^1}{\partial y^2} = 0\,, \tag{18}$$

$$\frac{\partial EA}{\partial y}\frac{\partial u^1}{\partial x} + 2EA\frac{\partial^2 u^1}{\partial x \partial y} = 0\,, \tag{19}$$

and

$$EA\frac{\partial^2 u^1}{\partial x^2} = 0\,. \tag{20}$$

Equation 18 can be rewritten as

$$\frac{\partial}{\partial y}\left(EA\frac{\partial u^1}{\partial y}\right) = -\frac{\partial}{\partial y}\left(\frac{EA}{l}u_l^0\right), \tag{21}$$

which can be integrated once and rearranged to yield

$$EA\frac{\partial u^1}{\partial y} + \frac{EA}{l}u_l^0 = C_3(x)\,. \tag{22}$$

Note that equation 22 states that a function of x and y (say $g(x,y) = EA\frac{\partial u^1}{\partial y} + \frac{EA}{l}u_l^0$) is equal to a function of x only (say $f(x) = C_3(x)$) for all x,y—this can imply that either $g(x, y)$ is a function of x only or both $g(x, y)$ and $f(x)$ are constant. The former does not lead to an immediate solution,* while the latter leads to the solution

$$C_3(x) = C_3, \quad u^1(x,y) = C_3\,\alpha(y) - \frac{y}{l}u_l^0 + C_4(x)\,, \tag{23}$$

where C_3 is a pure constant to be determined by the boundary conditions. The substitution of equation 23 into equation 19 and the enforcement of the resulting equation for all y determine that $C_4(x) = C_4$ (i.e., that C_4 is also a pure constant to be determined by the boundary conditions).† Note that the resulting solution for the microscale displacement u^1 is independent of x and satisfies equation 20 identically. Following application of equations 12 and 14, the microscale displacement is given by

$$u^1(y) = \frac{u_l^0}{\varepsilon\alpha(l/\varepsilon)}\alpha(y) - \frac{y}{l}u_l^0\,. \tag{24}$$

Due to the presence of the multiplier ε in equation 6, $\varepsilon\, u^1(y)$ is bounded for all y as $\varepsilon \to 0$. Note that the microscale displacement is not necessarily periodic in y even if the axial rigidity EA is. Traditional homogenization procedures summarily impose periodicity on the microscale displacement. As a final note, for the case of a homogenous rod (i.e., $EA^1(y) = 0$), equation 24 evaluates to zero, the macroscale displacement is given by equation 17, and the exact solution is recovered.

2.2 Extension of Procedure to Include Higher-Order Terms in $u^\varepsilon(x^\varepsilon)$

The solutions presented in section 2.1 were found by truncating the asymptotic expansion (equation 6) up to $O(\varepsilon^3)$. If instead truncation is not performed, a new term involving $u^2(x,y)$

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*Simplification of the equations does not occur for this choice, but the possibility of a second solution arising from this choice may exist.

†For the case of a nonzero external load $f(x)$, C_4 is replaced by $\frac{\int f(x)dx}{\partial EA/\partial y} + C_4$.

appears in equations 9 and 19. Similarly, new terms involving $u^2(x,y)$ and $u^3(x,y)$ appear in equations 10 and 20. Note that equation 10, and thus equation 20, were not used in developing the solution procedure but instead were checked for satisfaction. In the solution presented for this section, attention is therefore focused only on solving the new equation 19, namely

$$\frac{\partial EA}{\partial y}\frac{\partial u^1}{\partial x}+2EA\frac{\partial^2 u^1}{\partial x\partial y}+\frac{\partial}{\partial y}\left(EA\frac{\partial u^2}{\partial y}\right)=0, \tag{25}$$

with the still valid equations 22 and 23. In this manner, macro- and microscale displacements will again be developed without the need to first truncate the displacement asymptotic series given by equation 6.

Substituting equation 23 into equation 25 and redistributing yields

$$C_4' = \frac{-\dfrac{\partial}{\partial y}\left(EA\dfrac{\partial u^2}{\partial y}\right)}{\dfrac{\partial EA}{\partial y}}, \tag{26}$$

where a prime denotes differentiation with respect to x. Note that equation 26 states that a function of x (say $f(x) = C_4'$) is equal to a second function of both x and y (say $g(x,y) = -\frac{\partial}{\partial y}\left(\mathrm{EA}\frac{\partial u^2}{\partial y}\right)\Big/\frac{\partial \mathrm{EA}}{\partial y}$).

As in the previous section, a solution in which both $f(x)$ and $g(x,y)$ are the same constant is sought. This leads to the expression $C_4 = C_5x + C_6$ and an updated expression for $u^1(x,y)$,

$$u^1(x,y)=C_3\,\alpha(y)-\frac{y}{l}u_l^0+C_5x+C_6, \tag{27}$$

with three undetermined true constants. Application of the first boundary condition (equation 12) yields $C_6 = 0$, while the second boundary condition (equation 13) yields

$$C_3\,\alpha\left(\frac{l}{\varepsilon}\right)-\frac{1}{\varepsilon}u_l^0+C_5l=0. \tag{28}$$

Separating equation 28 into $O(\varepsilon^{-1})$ and $O(\varepsilon^0)$ terms yields two equations for the remaining constants:

for ε^{-1},

$$C_3\,\alpha\left(\frac{l}{\varepsilon}\right)-\frac{1}{\varepsilon}u_l^0=0; \tag{29}$$

and for ε^0,

$$C_5l=0, \tag{30}$$

which, when satisfied again, yields equation 24.

2.3 Application to an Example Rod—Linearly Varying Axial Rigidity *EA*

The new homogenization procedure described in section 2.1 is applied to a rod of unit length with a linearly increasing axial rigidity given by

$$EA = 3 + 0.01y\,, \tag{31}$$

and with an end displacement given by $u_l^0 = 0.1$. The microscale y is chosen to be one one-hundredth of the macroscale x such that $\varepsilon = 0.01$. This information, evaluated with the definition of $\alpha(y)$, the truncated expansion (equation 6), and the ordered displacements (equations 17 and 24), yields a predicted solution for the displacement field

$$u^\varepsilon(x^\varepsilon) = -0.382 + 0.348\ln(3 + x^\varepsilon)\,, \tag{32}$$

where all calculations have been carried out to three significant figures. For comparison, an exact solution exists for the linearly varying rod. Collecting the relevant information, the boundary value problem governing the rod's exact displacement field is as follows:

$$\frac{\partial}{\partial x}\left(EA\frac{\partial u}{\partial x}\right) = 0\,,\ EA = 3 + 0.01y\,,\ u(0) = 0\,,\ u(1) = 0.1\,, \tag{33}$$

which has the solution

$$u(x) = \frac{1}{10}\frac{\ln(3)}{\ln(3) - 2\ln(2)} - \frac{1}{10}\frac{\ln(3 + x)}{\ln(3) - 2\ln(2)}\,. \tag{34}$$

Evaluating equation 34 to three significant figures yields the exact displacement

$$u(x) = -0.382 + 0.348\ln(3 + x)\,, \tag{35}$$

which matches the perturbation solution (equation 32). The same match occurs when the calculations are carried out to any number of significant figures, indicating that for the linearly varying rod, the newly described homogenization procedure recovers the exact solution.

2.4 Application to an Example Rod—Periodically Varying Axial Rigidity *EA*

As a second example, the new homogenization procedure is applied to a rod of unit length with a periodically varying axial rigidity given by

$$EA = 3 + \sin(\frac{\pi y}{5})\,, \tag{36}$$

and with an end displacement given by $u_l^0 = 0.1$. The microscale y is chosen to be one one-hundredth of the macroscale x such that $\varepsilon = 0.01$ (note that this gives a y-period of 10 for the axial rigidity). This information, evaluated with the definition of $\alpha(y)$, the truncated expansion (equation 6), and the ordered displacements (equations 17 and 24), yields a predicted solution for

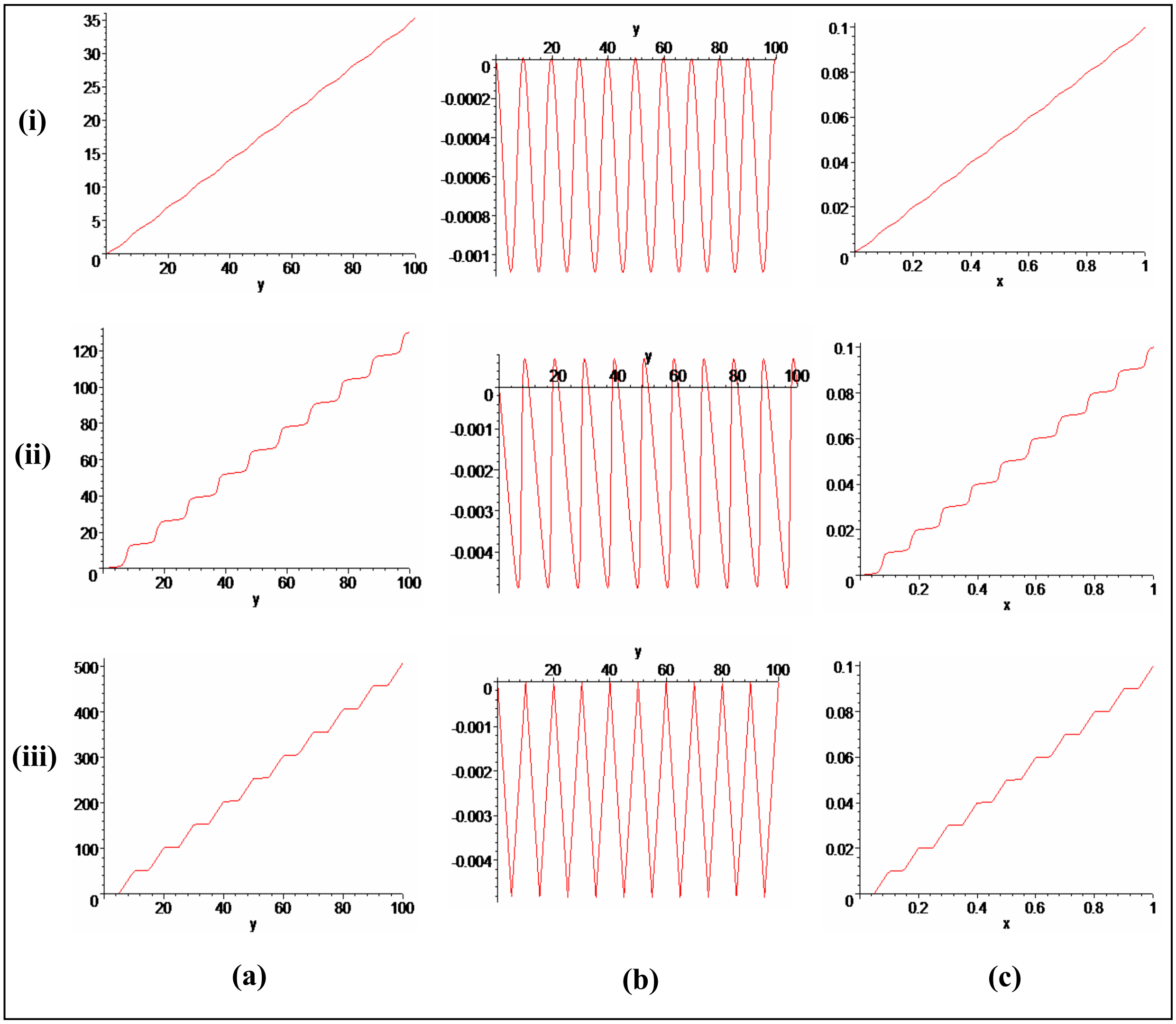

Figure 1. (a) The function $\alpha(y)$, (b) the microscale displacement field $\varepsilon u^1(y)$, and (c) the predicted displacement field $u^\varepsilon(x^\varepsilon)$ for the example rod with periodically varying axial rigidity (i) $EA = 3 + \sin(\pi y/5)$, (ii) $EA = 3 + 2.9\sin(\pi y/5)$, and (iii) $EA = 3 + 2.9\,signum(\sin(\pi y/5))$.

the displacement field. The top portion of figure 1 shows the results for the function $\alpha(y)$, the predicted microscale displacement field $\varepsilon u^1(y)$, and the predicted displacement field $u^\varepsilon(x^\varepsilon)$ for this example.

It is interesting to note from this example that the microscale displacement is indeed y-periodic, as imposed a priori in the traditional homogenization procedure. The effects of further increasing the variability of the axial rigidity are shown in the middle portion of the figure. Finally, the results for a rod with nonsinusoidal, but still periodic, axial rigidity are given in the bottom portion of the figure. This last example gives further evidence supporting the imposition of microscale displacement periodicity in the standard homogenization method (note that, indeed, the microscale displacement is periodic).

3. Conclusions

Using the well-established homogenization theory, a modification has been proposed for engineering applications in which the microscale displacement field is nonperiodic. The result is a novel nonperiodic homogenization procedure for functionally graded and reduced dimension problems where *y*-periodicity breaks down because of material or dimensional considerations. A specialized one-dimensional formulation was presented, verified against an exact solution, and subsequently demonstrated. A fully three-dimensional formulation is currently underway and will be presented in a sequel paper.

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1	INST FOR ADVNCD TCHNLGY THE UNIV OF TEXAS AT AUSTIN 3925 W BRAKER LN STE 400 AUSTIN TX 78759-5316
1	US MILITARY ACADEMY MATH SCI CTR EXCELLENCE MADN MATH THAYER HALL WEST POINT NY 10996-1786
1	DIRECTOR US ARMY RESEARCH LAB AMSRD ARL CS IS R 2800 POWDER MILL RD ADELPHI MD 20783-1197
3	DIRECTOR US ARMY RESEARCH LAB AMSRD ARL CI OK TL 2800 POWDER MILL RD ADELPHI MD 20783-1197
3	DIRECTOR US ARMY RESEARCH LAB AMSRD ARL CS IS T 2800 POWDER MILL RD ADELPHI MD 20783-1197

NO. OF COPIES	ORGANIZATION
	ABERDEEN PROVING GROUND
1	DIR USARL AMSRD ARL CI OK TP (BLDG 4600)

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